

=> fil reg

FILE 'REGISTRY' ENTERED AT 10:45:09 ON 16 SEP 2002  
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*Structure 5b*

STRUCTURE FILE UPDATES: 15 SEP 2002 HIGHEST RN 451445-11-7  
DICTIONARY FILE UPDATES: 15 SEP 2002 HIGHEST RN 451445-11-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STN Note 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d que 11;d que 12

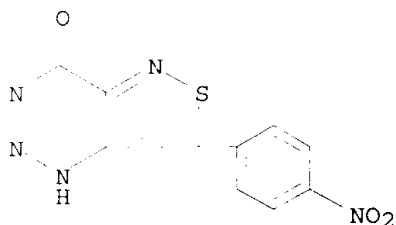
L1 44 SEA FILE=REGISTRY ABB=ON PLU=ON NSC3-N3C3/ES

L2 4 SEA FILE=REGISTRY ABB=ON PLU=ON 333.1144/RID

=> d 12 ide can 1-4

*Ly more match  
cleaned structures*

L2 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2002 ACS  
RN 72633-09-1 REGISTRY  
CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-(4-nitrophenyl)- (9CI) (CA  
INDEX NAME)  
FS 3D CONCORD  
MF C10 H5 N5 O3 S  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)



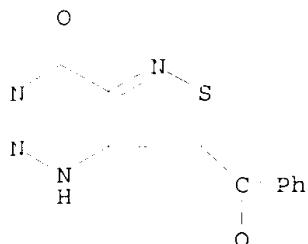
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

L2 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS

RN 72632-96-3 REGISTRY  
 CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-benzoyl- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C11 H6 N4 O2 S  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
 (\*File contains numerically searchable property data)

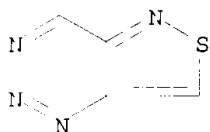


\*\*PROPEFTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

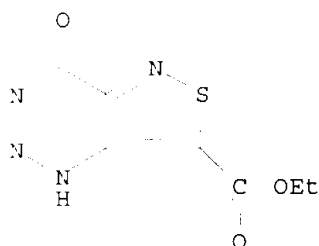
L2 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS  
 RN 55402-82-9 REGISTRY  
 CN Isothiazolo[4,3-d]-1,2,3-triazine (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C4 H2 N4 S  
 CI RPS



\*\*PROPEFTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS  
 RN 54968-80-8 REGISTRY  
 CN Isothiazolo[4,3-d]-1,2,3-triazine-7-carboxylic acid, 1,4-dihydro-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C7 H6 N4 O3 S  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
 (\*File contains numerically searchable property data)

*Handwritten notes:*  
 1529 (190)  
 1529 (190)  
 1529 (190)  
 1529 (190)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1967 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

REFERENCE 2: 82:139991

=> fil hcaplus  
FILE 'HCAPLUS' ENTERED AT 10:47:16 ON 16 SEP 2002  
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FILE COVERS 1907 - 16 Sep 2002 VOL 137 ISS 12  
FILE LAST UPDATED: 15 Sep 2002 (20020915/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.  
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> s l2

L3 2 L2

=> d .ca 1-2

L3 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1980:76382 HCAPLUS

DOCUMENT NUMBER: 92:76382  
 TITLE Synthesis and reactions of 4-aminoisothiazoles  
 AUTHOR(S): Gewald, Karl; Bellmann, Peter  
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027,  
 Ger. Dem. Rep.  
 SOURCE Liebigs Ann. Chem. (1979), (10), 1534-46  
 CODEN: LACHDL  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB 4-MeC6H4ON:CRCN (R = CONH2, CO2Et, CPh, Ph, 4-O2NC6H4) reacted with  
 R1CH2SH (R1 = CPh, CO2Et, COMe, CO2H, C6H4NO2-4, CHO, Ph) to give the  
 corresponding aminoisothiazoles I via the intermediates R1CH2SN:CRCN.  
 Decarboxylation gave 5-unsubstituted 4-aminoisothiazoles, e.g., reaction  
 of I (R = CONH2, R1 = CO2Et) with HCl gave 3-carboxy-4-aminoisothiazole,  
 which was heated with Ac2O to give 4-acetamidoisothiazole. I were also  
 converted into the ring systems II (R1 = CPh, CO2Et, C6H4NO2-4), III (R1  
 = CO2Et, COMe), IV (R = CONH2, Ph, C6H4NO2-4), and V (R = CONH2, CO2Et; R2  
 = H, Me).  
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 54968-79-5P **54968-80-8P** 72632-83-8P 72632-86-1P  
 72632-88-3P 72632-91-8P 72632-92-9P 72632-93-0P 72632-94-1P  
 72632-95-2P **72632-96-3P** 72632-97-4P 72632-98-5P  
 72632-99-6P 72633-00-2P 72633-01-3P 72633-02-4P 72633-03-5P  
 72633-04-6P 72633-05-7P 72633-06-8P 72633-08-0P **72633-09-1P**  
 FL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

L3 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1975:139991 HCAPLUS  
 DOCUMENT NUMBER: 82:139991  
 TITLE: New syntheses of 4-aminoisothiazoles  
 AUTHOR(S): Gewald, Karl; Bellmann, Peter; Jaensch, Hans J.  
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, E. Ger.  
 SOURCE: Z. Chem. (1975), 15(1), 18-19  
 CODEN: ZECEAL  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB Aminoisothiazoles I (R = CONH2, CO2Et; R1 = CO2Et, Ac) were prepd. in 48  
 60% yield by treating NCCR:NO3SC6H4Me-p with R1CH2SH in the presence of  
 base at <40.degree.. H2NCOC(CN):NSCH2CO2Et was also isolated and  
 diazotized, giving the isothiazolotriazinone II (X = N). Condensation of  
 I (R = CONH2, R1 = CO2Et) with HC(OEt)3 gave II (X = CH).  
 CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 54968-75-1P 54968-76-2P 54968-79-5P **54968-80-8P**  
 FL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)